

---

**UK Consortium on Turbulent Reacting Flows  
(UKCTRF): EP/R029369/1:  
4<sup>th</sup> Annual Meeting**

**Nilanjan Chakraborty**

School of Engineering

Newcastle University, Claremont Road, Newcastle-Upon-Tyne, NE1 7RU



**1<sup>st</sup> of December 2021**

---

# Outline

---

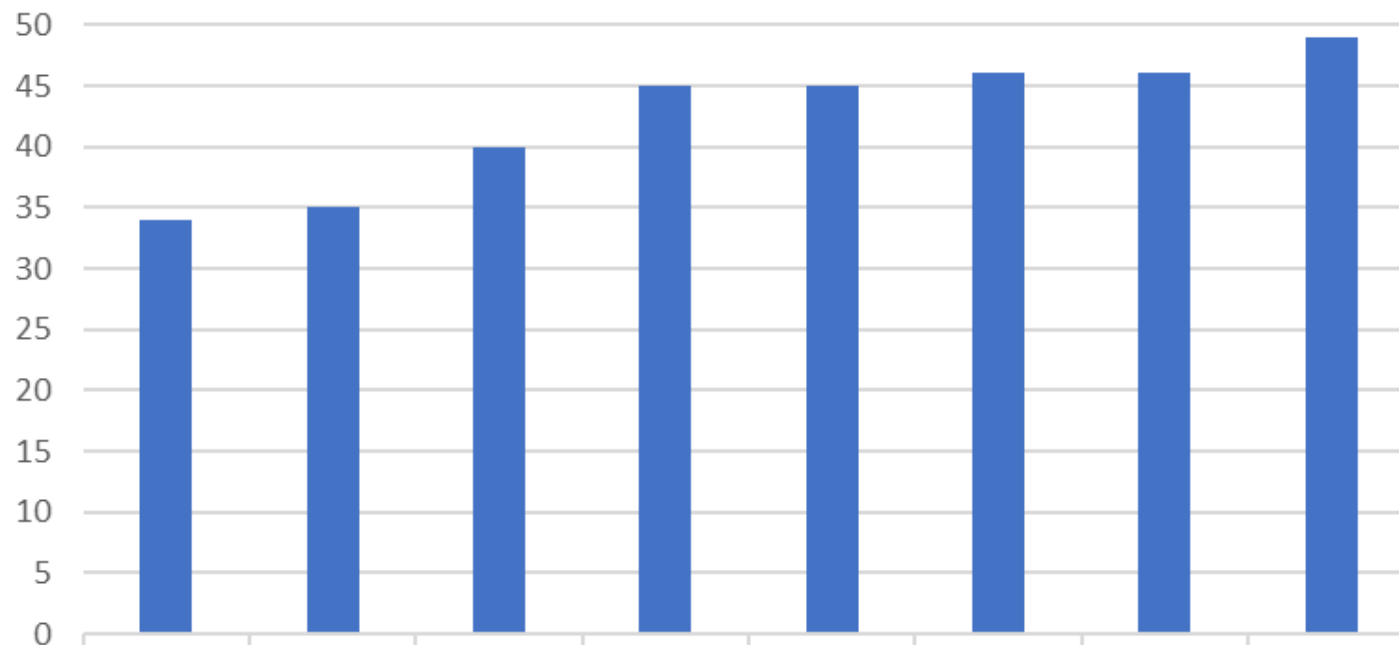
- Demands and availability of computational time
  - Application for computational time allocation
  - Updates on computational architecture
  - Current usage of computational time allocation
  - Travel funding by consortium
  - Annual progress report
  - ExCALIBUR update
  - UKCTRF updates
  - Final comments
-

# Demand and availability of computational time



# Evolution of member number of the UKCTRF

UKCTRF Members



	2013 - 2014	2014 - 2015	2015 - 2016	2016 - 2014	2017 - 2018	2018 - 2019	2019 - 2020	2020 - 2021
■ Member Numbers	34	35	40	45	45	46	46	49

# Application for computational time allocation

---

- Application form is available on <http://forms.ncl.ac.uk/view.php?id=5420>
  - Review process & review panel (UKCTRF management team)
  - Queries are dealt within 48 hours
  - Decision is made typically within 10 days
  - We do not accept more than 2 applications from a particular named investigator's group
  - Demand is higher than availability and we will be more discerning before awarding the computational time in the future
  - Any feedback to improve the process or make it better
-

# Update on computational infrastructure

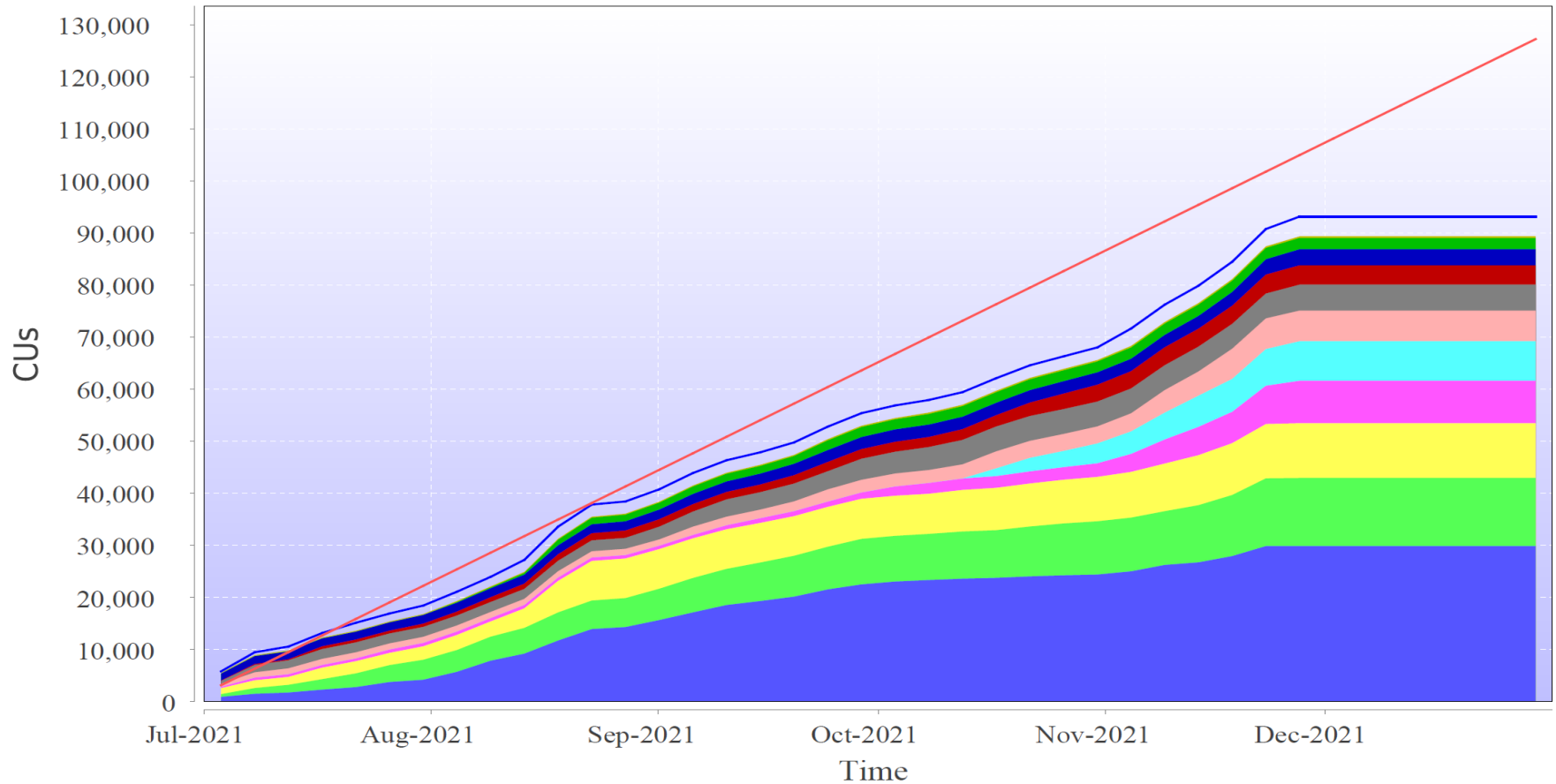
---

- The remaining allocation for our consortium for the 4-cabinet service will continue to run through December 2021 but usage of this service will come out of the current allocation amount..
  - The initial period of access for the full ARCHER2 service will be charge free until early January. At this time, it will move to the usual charging.
  - Consortia allocation for the first six-month period (Jan – July 2022) is available on SAFE. The applications for the computational time will be invited soon.
  - The applicants need to justify their requests and they should not rely on the historical computational time allocations for their projects. This is especially important for the projects which fall in the periphery of the remit of this consortium.
  - The members are not expected to request computational times for the same project from more than one consortia, but it needs to be declared if there is a good justification for doing so.
  - It is very important that disk space is properly managed. Please delete the old files which are not used. Serial offenders might not be allowed to run jobs on ARCHER2.
-

# Current usage of computational time allocation

Percentage of allocation used: 71%

Percentage of time elapsed: 82%



# Travel funding by consortium

- Each named investigator's group £500 was allocated for each PI's group for orally presenting a paper at other conferences other than combustion symposium. This will be revisited later tomorrow in the management team meeting.
- We received 4 applications for contributions to the cost of registration/travel to the 13<sup>th</sup> European Turbulence Modelling and Measurements (ETMM-13) conference resulted from the UKCTRF activities. All those made applications are requested to send the invoice to Mrs. Joanne Redshaw ([joanne.redshaw@newcastle.ac.uk](mailto:joanne.redshaw@newcastle.ac.uk)) as soon as possible if it is not already done.
- The papers for which travel funding will be provided will need to meet the following requirements:
  - **It needs to deal with reacting flows. If the paper is on laminar flows, it must have some relevance to turbulent reacting flow modelling**
  - **It needs to explicitly acknowledge ARCHER and consortium grant (EP/R029369/1)**



# Consortium website ([www.ukctrf.com](http://www.ukctrf.com))

Please be familiar with the consortium website:

- Application forms for reimbursement, travel funding and computational time application are available

(<http://www.ukctrf.com/index.php/reimbursement/>, <http://www.ukctrf.com/index.php/travel-funding/> , <http://www.ukctrf.com/index.php/computer-time-allocation/> )

- List of sample publications by the consortium members

([http://www.ukctrf.com/wp-content/uploads/2018/12/Sample-Publications-for-Website\\_24.08.2017.pdf](http://www.ukctrf.com/wp-content/uploads/2018/12/Sample-Publications-for-Website_24.08.2017.pdf) )

- List of the travel grants for PhD students and RAs

(<http://www.ukctrf.com/index.php/conference-funding/> )

- List of presentations given in earlier meetings, annual reports and case studies are available on the website

(<http://www.ukctrf.com/index.php/events/> )

- Information on the flagship codes of the UKCTRF can be obtained

from:(<https://www.ukctrf.com/index.php/senga/>, <https://www.ukctrf.com/index.php/hamish/> )

# Annual progress report & Impact capture

---

- A survey will open soon after this meeting. This survey is expected to capture all the impacts that this consortium made since its inception in 2014. This is critical for making a case for our renewal. Please fill up the survey and try your best to provide the requested information. A failure to complete the survey within the deadline will automatically disqualify computational time applications.
  - EPSRC expects an extensive report and a minimum of 3 case studies based on our annual activities. We will need volunteers for these case studies. The annual reports and case studies can be found on: <https://www.ukctrf.com/index.php/impact/>
  - We will need list of publications, list of grants and prizes and case studies from the consortium members for the next annual progress report and future Researchfish submissions. Please provide the necessary information within the deadline.
-

# ExCALIBUR (<https://excalibur.ac.uk/excalibur> )

- ExCALIBUR stands for **Exascale Computing Algorithms and Infrastructures Benefitting UK Research**
- £45.7M initiative from the UK government's [Strategic Priorities Fund](#) (SPF)
- Led by the [Met Office](#), [UK Research and Innovation](#) (UKRI) with the [UK Atomic Energy Authority](#) (UKAEA)
- The UK's Exascale Programme for the next 5 years (started November 2019)
- Focus on software and algorithms
- Funding breakdown: EPSRC - £22.8M, Met Office / UKAEA - £17.0M, Hardware and Enabling Software (H&ES) - £4.5M
- The intended outcomes are [Knowledge integration](#); [High priority use cases](#); [Emerging requirements for HPC algorithms](#); [Cross-cutting research](#); [Proof-of-concept hardware \(H&ES\)](#)

# UKCTRF updates (1)

- A multi-institutional (involving Cambridge, Newcastle, Imperial, Southampton, Warwick) EPSRC bid totalling £3M has turned out to be successful in response to ExCALIBUR Phase 1b call. This project will bring together (for the first time) communities representing two of the seven UK [HEC Consortia](#), the [UK Turbulence Consortium](#) (UKTC) and the [UK Consortium on Turbulent Reacting Flows](#) (UKCRF) , to re-engineer or extend the capabilities of four of their production and research flow solvers for Exascale computing: [Xcompact3d](#), [OpenSBLI](#), [uDALES](#) and [SENGA+](#).
- These open-source, well-established, community flow solvers are based on finite-difference methods on structured meshes. We consider is the best strategy to achieve performance at scale (no meshing issues, no load balancing issues, possibilities to limit data movement & global communications, wide range of options to optimise bandwidth and memory usage, such as memory tiling and near-neighbour communications). A key aim of this project is to leverage the well-established Domain Specific Language (DSL) framework [OPS](#) and the [2DECOMP&FFT](#) library to allow Xcompact3d, OpenSBLI, uDALES and SENGAs to run on large-scale heterogeneous computers.
- An application is made in response to UKRI's ExCALIBUR cross-cutting call on **Evolutionary Re-Engineering of Multi-Physics Fluid Flow Solvers with embedded DSLs for Exascale Computing** in collaboration with UKTC (Dr. Sytvain Laizet, Imperial College), Warwick University (Dr. G. Mudalige), STFC, Met Office. We are waiting for the outcome.

# UKCTRF updates (2)

---

- An application is made in response to EPSRC's Software for Research Communities call on the theme of development and re-engineering of existing software. This call focuses on transfer of capabilities from OpenFOAM to Code\_Saturne. This application is also made in collaboration with UKTC. The bid is led by Dr. C. Moulinec from STFC, and there are Co-Is from Manchester, Newcastle and Warwick. The proposal is currently under review.
  - UKCTRF members are strongly encouraged to take part of the knowledge exchange activities of the ExCALIBUR programme. It will provide future opportunities of collaborative research involving software development for future Exascale machines and hybrid infrastructure.
  - An ARCHER2 pioneer project on large-scale DNS of Flame-Wall Interaction of Hydrogen-air flames in turbulent boundary layer was successful in 2020. This project will start as soon as ARCHER2 is available in its full capacity.
  - The call for High End Computing consortia renewal will be issued soon. The community needs to be prepared for the bid.
-

# Workplan and future meetings

█ : (Proposed activity at the desired level); 
 █ : (Proposed activity for reduced resource); 
 █ : Activity in Flagship Software grant (EP/P022286/1)

Phases \ Quarter	1 1	1 2	1 3	1 4	2 1	2 2	2 3	2 4	3 1	3 2	3 3	3 4	4 1	4 2	4 3	4 4	Milestones/ Deliverable	
I. initial allocation for HPC time and continuation of UKCTRF activities in WP1 & WP2					◀ M1												↻ M1 (Year 1 report)	
II. Code development and initial validation for new capabilities WP1 and WP2								◀ M2										
III. Production level runs for WP1 and WP2 using HPC facilities																	↻ M2 (Year 2 report)	
IV. Algorithm and architecture development for future platforms in WP 3c + WP 3d																		
V. Validation & documentation of SENG+ and HAMISH and new release of SENG+ (WP3a & 3b)													◀ M3					↻ M3 (Year 3 report)
VI. Website development and maintenance																		
VII. Dissemination																◀ M4	↻ M4 (Year 4 report)	
Progress markers	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑		
	R1 Kick-off meeting (Year 1)	R2 Annual progress meeting (Year 1)			WS1:Workshop 1 + R3 Annual progress meeting (Year 2)				R4 Annual progress meeting (Year 3)							WS2:Workshop 2+ R5 Final Meeting (Year 4)		
	Initial planning of utilisation of computational time	Year 1 Interim Report			Year 2 Interim Report				Year 3 Interim Report							Year 4 Final Report		↻ Deliverable

Jan 19

Jan 20

Jan 21



Jan 22

Jan 23

We are here

# Final comments

---

- The final meeting of this funding cycle will take place at Newcastle University on the **13<sup>th</sup> -14<sup>th</sup> of September 2022**. The meeting will be organized as an international conference.
  - There will be a **special issue in Flow, Turbulence and Combustion** based on the UKCTRF activities after the final meeting. All the members of the UKCTRF and impact advisory panel members are invited to submit to this special issue. The deadline will be at the end of November 2022. More information will follow closer to the time in 2022.
  - The named investigators of the UKCTRF to request their users to clean the disk space on ARCHER as it is stopping people to use the resources.
  - We would like to thank all the Impact Advisory Panel members for devoting their valuable time. Special thanks are due to the plenary lecture speakers for their time and effort.
  - I am also grateful to the session chairs for their support, and finally I would like to thank our local organiser Dr. Jun Xia for all his help. I am also grateful to Mrs. Joanne Redshaw for her administrative help.
-